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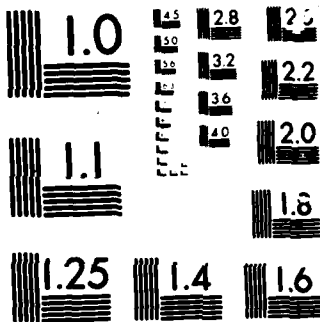
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ABSTRACT

This document presents a computational system designed to remove known components from spectroscopic data. The system realization is a FORTRAN-77 program; a listing of the program's source code is included in the Appendix.

The program first performs a nine-point quadratic least-squares smoothing function. It then removes the known component with a non-recursive filter based on a least-squares prediction of the observed spectrum and a least-squares prediction of a computer generated synthetic spectrum of the known component.

The program was tested using an artificial spectrum created for the sole purpose of testing the program's function.

The program's function was verified with three segments of the 12 micron band of ethane taken from data recorded on the Fourier transform spectrometer at the McMath solar telescope at the Kitt Peak National Observatory. The segments are located near 804.0, 815.0, and 819.5/cm⁻¹. Plots of the spectral data and of the resultant data are included.

A DIGITAL FILTER FOR REMOVING KNOWN
COMPONENTS FROM SPECTROSCOPIC DATA

A Thesis
Presented for the
Master of Science
Degree
The University of Tennessee, Knoxville

Carey G. Mumford III

August 1985

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CHAPTER I

INTRODUCTION

The purpose of this study is to devise a technique whereby any known component of a given spectrum can be removed to enable study of the underlying spectral data without interference from the unwanted component. The program embodying the developed technique, called FILTER, first carries out a quadratic least-squares smoothing operation on the spectrum being studied. Following a mild smoothing operation, a non-recursive least-squares filter is applied to the observed spectrum. This filter is constructed from the predicted synthetic spectrum of the component to be removed. The output of the filter may be thought of as an "error spectrum" which reflects the least-squares difference between the observed complete spectrum and the synthesized component upon which the filter is based.

Often in the study of spectroscopic data, one is interested in features that are so near other larger features that information about the feature in question is very difficult to obtain. Without some method of removing the large features, the small ones are mostly inaccessible. Of course, it is not necessary that the desired feature be a small one. One may wish to separate

two equivalent sized components or remove a known small component that is distorting the data to be studied.

For instance, in the study of ion spectra, any given transition is extremely weak (Saykally, 1984). Unless the transition is fortuitously isolated, it may not be observable. In the case of infrared molecular spectroscopy of isotopic molecules, some transitions are separated from their relatives by less than a milliwavenumber (10^{-3} cm^{-1}). Clearly, any analysis of the spectrum would be complicated by the nearby transitions. The structure of planetary atmospheres can be determined through the use of spectroscopy, but many transitions--and consequently many atmospheric constituents--can not be identified because of their proximity to other spectral lines. By using FILTER, one can remove selective portions of an observed spectrum to isolate the desired features for more detailed study.

Another potential use of this program, and the one which this work addresses, is in the study of hot-band spectra which normally are intermixed with the cold-band spectra and consequently are difficult to pick out of the data. With FILTER, one can eliminate the known ground-state transitions from the observed spectrum leaving the smaller hot-band features in a prominent position to be studied.

The program itself is a simple, yet elegant, approach to a complex problem. It uses a nine-point least-squares smoothing routine to reduce the effect of noise. After smoothing, it uses the calculated synthetic spectrum to develop a predicted component of the observed spectrum and perform a non-recursive filtering function. Once the smoothing/filtering function is complete, a simple point-by-point subtraction leaves the error spectrum in the resultant data file.

The data files must first be processed so that they represent the same arrangement of information--data-point density, line widths and so forth must be equivalent or the results will be meaningless. Though the manipulation of the data files required to achieve such a suitable arrangement for input to the program represents an additional effort in the analysis of the spectrum, the additional information available in the residual spectrum more than compensates for the extra work.

The discussion in this work is geared toward infrared spectroscopy and the test runs were accomplished using infrared spectra--specifically of the ν_3 band of ethane, but the program is easily adaptable to any spectroscopic data.

CHAPTER II

BACKGROUND

In the course of any spectroscopic analysis, one will encounter several concepts; in order to understand the workings of FILTER, one needs to be familiar with some basic ideas.

In infrared molecular spectroscopic theory (Herzberg, 1945) line positions and intensities are the primary data used to obtain physically useful and meaningful results. Once position and intensity have been accurately established, the contribution of line shape to the spectral data becomes important too. In addition to infrared theory, one should understand the process of deconvolution (Blass and Halsey, 1981) and have a good grasp of the data processing techniques used to manipulate the spectra (Pennington, 1970). The use of the filtering scheme in the program is constrained by the digital data-processing techniques used in the program (Bozic, 1979). When one is knowledgeable of these concepts, the validity of the resultant data follows.

Molecular Vibration-Rotation Theory

The physical model used in characterizing molecular vibration-rotation energy levels is straightforward

but complex. Since this project was only peripherally involved with the concepts, a brief summary is presented.

One considers a molecule as a polyatomic system of N nuclei and n electrons. The system then has $3(N+n)$ degrees of freedom. The Born-Oppenheimer approximation allows one to separate the contribution of the electronic motion, so only $3N$ degrees of freedom need be considered. Furthermore, it is always possible to separate the three degrees of freedom that correspond to the motion of the center-of-mass. The remaining $3N-3$ degrees of freedom cannot be separated easily, but by assuming the molecule is a rigid rotor, one can assign a body-fixed frame of reference and separate the rotational motion from the vibrational motion (Herzberg, 1945).

Line Position

This body-fixed frame of reference allows one to assume a linear combination of the vibrational and rotational Hamiltonians. The determination of molecular energy, then, is a combination of two problems.

The solution of the rotational Hamiltonian leads to an expression for the rotational energies of the molecule:

$$F(J,K) = BJ(J+1) + (A-B)K^2 \quad (1)$$

where J and K are the rotational quantum numbers and the

rotational constants are

$$B = \frac{h}{8\pi^2 c I_B}, \quad A = \frac{h}{8\pi^2 c I_A}. \quad (2)$$

Similarly, the solution of the vibrational Hamiltonian leads to an expression for the vibrational energies of the molecule:

$$G(v_1, v_2, \dots) = \omega_1(v_1 + 1/2) + \omega_2(v_2 + 1/2) + \dots \quad (3)$$

where v_n are the vibrational quantum numbers of the n th normal mode of vibration and ω_n are the frequencies of the normal vibrations (Herzberg, 1945).

Unfortunately, the rigid-body approximation does not give sufficient accuracy for high resolution spectroscopy. To correct for the non-rigidity of the molecule, two changes are needed. First, the coefficients are changed slightly from the equilibrium values used in the rigid-body approximation to a value that accounts for the average motion. Second, some additional terms are added to the expressions to account for factors such as anharmonicity, distortions of the molecule and coriolis effects. The energy expressions are rewritten:

$$F^V(J, K) = B^V J(J+1) + (A^V - B^V) K^2 - (A \xi_t) K l_t - D_J^V J^2(J+1)^2 - D_{JK}^V J(J+1) K^2 - D_K^V K^4 \quad (4)$$

and

$$G(v_1, v_2, \dots) = \sum_i \omega_i (v_i + 1/2) + \sum_i \sum_{k>i} x_{ik} (v_i + 1/2)(v_k + 1/2) + \dots \quad (5)$$

where the v superscript indicates an average value, the D 's are centrifugal distortion constants, the $(A \xi_t)$ is a coriolis constant and the x_{ik} are corrections for anharmonicity. The total vibration-rotation energy of a molecule is then

$$T = G(v_1, v_2, \dots) + F^V(J, K) \quad (6)$$

and the line position or frequency follows from the energy difference (Herzberg, 1945).

The literature shows that a good study of most spectra will yield accuracy of the transition coefficients to within approximately .01%, so this first element of the computer program has a good foundation and one should reasonably expect FILTER to give accurate results in line positions.

Line Intensity

Line intensity is not so simple to calculate as line position. The approximations used in calculating line intensity are more susceptible to inaccuracy than those used in calculating the line position. These approximations can lead to proportionately larger errors

in the calculated theoretical intensity than should be encountered in calculating line position (Demtröder, 1981).

Quantum mechanically, the strength of a given transition is proportional to the square of the transition probability (Demtröder, 1981). Unfortunately, the literature is generally unclear in describing calculated line strengths, leaving guess work or trial-and-error as the primary tool in determining what has been included in the calculation of the line strength. In general, the calculated line strength must be scaled by some conversion factor to arrive at the absolute line strength.

Given the absolute line strength, one convolves the calculated line strength with the expected line shape, which is described below, to get the absorption coefficient.

The calculated absorption coefficient can then be used in the expression for transmitted intensity, T :

$$T = I_0 e^{-\alpha P l} \quad (7)$$

where I_0 is the incident intensity; α , the absorption coefficient; P , the pressure in atmospheres; and l , the path length in cm. This expression for T is derived from Beer's law for linear absorption (Demtröder, 1981). The absorptance obtained is then

$$A = 1.0 - T = 1.0 - I_0 e^{-\alpha Pl}. \quad (8)$$

The absorptance space obtained with this expression is the most accurate space available for analyzing strongly absorbing lines in a spectrum.

The absorption spectrum is sometimes analyzed in the absorption coefficient space obtained by a Taylor series of the expression for the absorptance which yields

$$A = \alpha Pl - \frac{(\alpha Pl)^2}{2!} + \dots \quad (9)$$

In the first approximation of this Taylor series, when αPl reaches 25%, the error in calculated line intensity is at least 3%. Clearly, whether to analyze the spectrum in absorptance space or in absorption coefficient space is dependent upon the maximum absorption expected in the spectrum.

Finally, the line shape has not yet been included in the calculation of line intensity. As will be seen below, the line shape used in determining the theoretical spectrum will also affect the intensity of the peaks in the calculated spectrum.

Line Shape

The expected line shape is equally as important as the line strength in calculating the theoretical spectrum. It affects the calculated line intensity during

the convolution process. Furthermore, the shape of the expected instrument function will also affect the calculated intensity.

In general, the intensity of a given line will decrease during convolution with a normalized profile because the convolution increases the width of the line. The overall problem of selecting a line shape and convolving that line shape with the stick spectrum contains many factors which will alter the intensity of the theoretical spectrum.

The actual line shape is taken to be a combination of several factors. The natural line profile is a Lorentzian. It is on the order of a few kHz and for the purposes of this study it can be approximated by a delta function (Demtröder, 1981). The doppler line width is represented by a Gaussian whose full width at half maximum (FWHM), Δ_D , is a function of the temperature of the sample:

$$\Delta_D = 7.16 \times 10^{-7} \nu_0 \sqrt{T/M} \text{ (cm}^{-1}\text{)} \quad (10)$$

where T is the temperature in °K and M is molecular mass in amu. Likewise, the observed line profile includes a contribution due to the pressure of the sample. The pressure broadening can be represented by a Lorentzian with FWHM Δ_p :

$$\Delta_p = 0.250P \text{ (cm}^{-1}\text{)} \quad (11)$$

where P is the pressure in atmospheres (Blass, 1985).

Both the doppler width and the pressure width must be taken into account when calculating the expected line shape of the sample to be studied. The resultant line shape is then convolved with the calculated stick spectrum to get the theoretical absorption coefficient spectrum. In absorptance space, the calculated spectrum can be expressed

$$A = 1 - e^{-(D \otimes P)SP_l} \quad (12)$$

where \otimes indicates a convolution function, D is the doppler width profile, P is the pressure width profile, S is the absolute line strength, and Pl is the pressure-path length product of the sample. The absorption coefficient, α , then is the convolution of D and P times S.

Deconvolution

In addition to the "real" line-shape factors mentioned in the previous section, one must also consider the instrument function when working with spectral data. After the theoretical absorptance spectrum has been determined, the expected instrument function is convolved with the theoretical absorptance spectrum to generate a

calculated synthetic spectrum containing known components.

The observed spectrum necessarily contains the instrument transfer function, which broadens the observed line width, effectively reducing the resolution. Deconvolution is a technique that can be used to increase apparent resolution or reduce required observing time by removing the instrument function from the observed data. The accuracy of the deconvolution process is highly dependent on a signal to noise ratio of 100 or better (Blass and Halsey, 1981).

Filtering

The digital spectral data may be filtered either as it is taken or it may be recorded in raw form and filtered in the process of analysis. The latter approach offers the advantage of safety and flexibility. If the data were to be filtered as it were taken, it could be catastrophically altered as a by-product of the filtering. By recording the data before filtering, one may always start over if non-physical results are achieved. Furthermore, more than one filtering method may be used if the results are not suitable.

One may work with either continuous-time or discrete-time data. Continuous-time refers to a data set in which the independent variable may assume a continuous

range of values while discrete-time implies that the independent variable is restricted to a finite discrete set of values. A discrete-time signal is often referred to as a sampled data signal (Freeman, 1965).

The digital signal may have data points taken at any of the discrete values of the independent variable. These values are usually equally spaced, however equal spacing is not a requirement. The data processing is considerably simpler with equal spacing (Bozic, 1979). In the discrete-time system, the independent variable time, t , is taken as

$$t=kT$$

where T is the difference between any two adjacent data points and k corresponds to the k th data point. The notation used in this work is $x(k)$ and $y(k)$ for the k th value of the independent and dependent variables respectively.

The process of filtering involves predicting a data point based on a number of input data points. It usually consists of applying some operation such as delay or multiplication by a constant to the input data points. If the filter uses past output as input, it is called recursive, while if it uses no past output, it is called non-recursive or moving average. The recursive filter has

some problems with stability and was not considered for this study (Bozic, 1979).

The general representation of a digital filtering scheme is

$$y(k) + b_1y(k-1) + \dots + b_my(k-m) = a_0x(k) + a_1x(k-1) + \dots + a_nx(k-n) \quad (13)$$

where $x(k)$ represents the k th input point; $y(k)$, the k th output point; and the a_n 's and b_m 's are weighting factors with b_0 taken as unity (Bozic, 1979). This representation means that at time k ($t=kT$) the output of the filter is the current input plus some linear combination of previous inputs and outputs. In the case of using recorded data, one may also include future inputs and outputs. For the non-recursive filter all b_m , $m>0$, are zero. Figure 1 is a generalized depiction of a recursive filter while Figure 2 illustrates a non-recursive filter.

Digital Processing

Use of poor technique in digital data processing can lead to catastrophic alteration of the data; hence, one must be alert not to generate excessive errors in processing the data. There are two factors in digital data processing that can contribute to the error: quantization and finite word length.

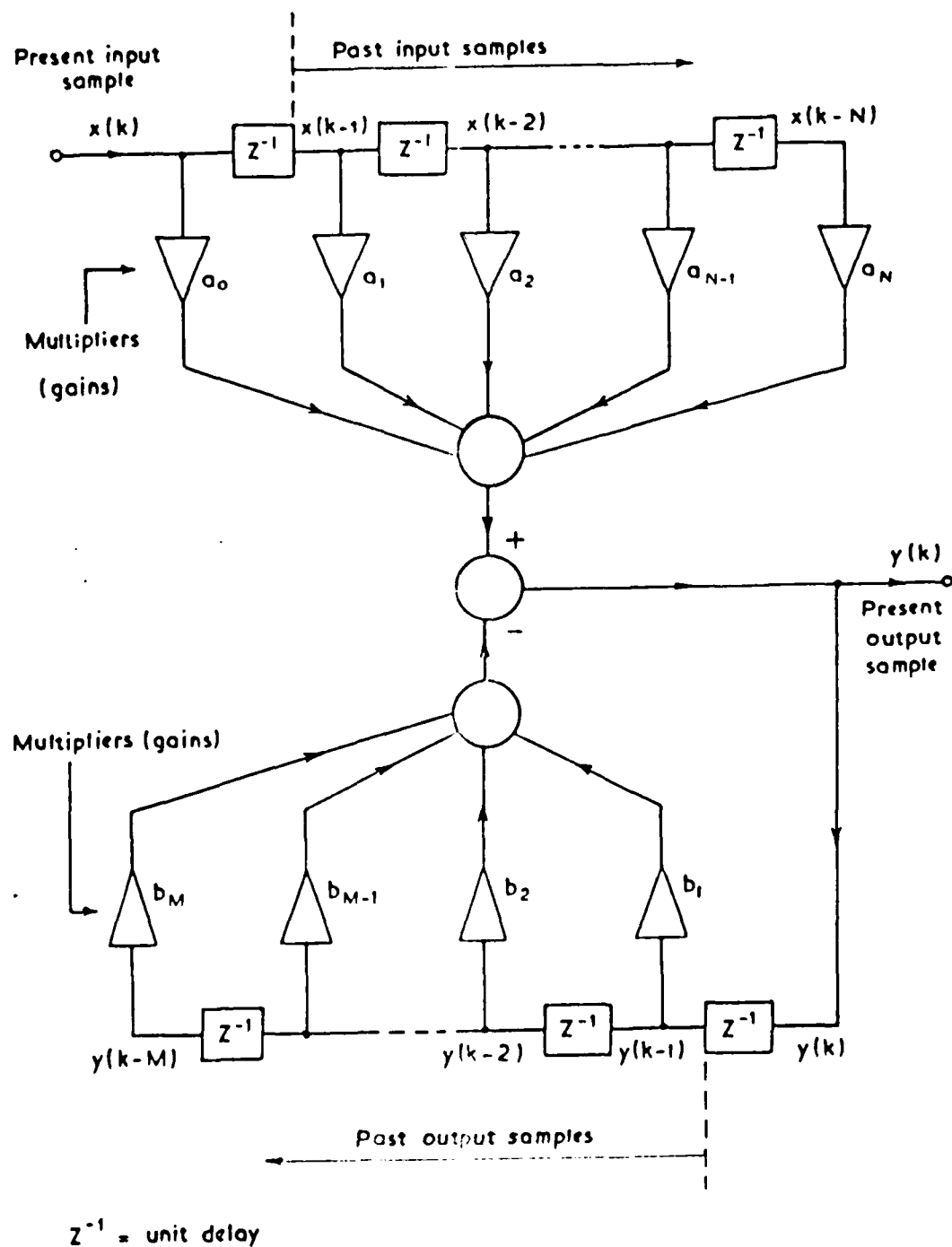


Figure 1. Diagram of a recursive filter.

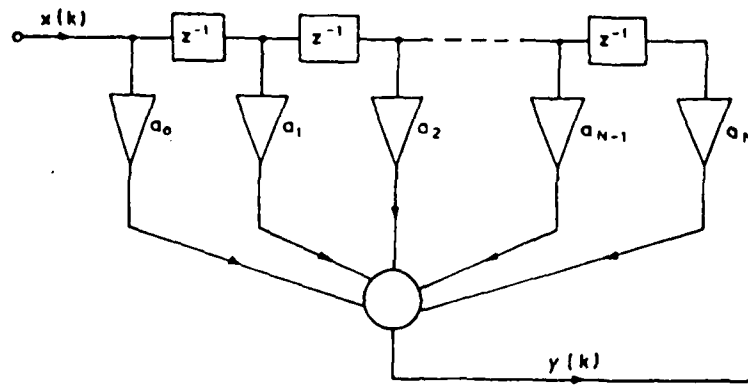


Figure 2. Diagram of a non-recursive filter.

Quantization error results from trying to describe infinite precision data with finite precision. The position or value of a data point will never precisely coincide with the discrete value available to describe it. Furthermore, there is some quantization error involved in the original measurement of the spectrum, but that is beyond the scope of this study. The slight inaccuracies involved in quantization error will appear as noise in the spectrum.

Finite word length errors will result in a loss of accuracy and generate apparent random noise when the result of any operation exceeds the precision of the computer. As a simple example, assume the computer can store only five digits plus the exponent. Then let $x = 1.4345 \times 10^6$ and let $y = 1.7332 \times 10^7$. When x is added to y , the result is 18,766,500, but the result will be

stored as 1.8766×10^7 and the information that the number is actually larger by 500 will be lost.

These errors are cumulative and the effect can be much larger than the one given in this example. Two procedures are useful in minimizing the effect of finite word length errors: avoiding subtraction of a large number from another large number and multiplying by factors less than one whenever possible (Pennington, 1970).

CHAPTER III

DESCRIPTION OF THE PROGRAM

FILTER is written in FORTRAN-77. An attempt was made not to use machine-specific code so that the program can be used on other machines with only minor alteration, however, the data files are identified to the program through interactive input/output. If interactive input/output is not possible, the source code must be modified to provide identification of the spectra to be used. The source code for FILTER is listed in the Appendix.

The spectrum files are formatted in double precision format with each point written as D20.12. The starting frequency of the spectrum is the first entry in the file and the step size is the second. Following the starting frequency and the step size, the spectral intensities are written to the file. The file must be written for random access input/output. If the data-point density and starting frequency of the calculated spectrum and the observed spectrum are not identical, the calculated spectrum must be altered in order to coincide with the observed spectrum.

The program uses a buffered input/output capability to handle large data files without using a prohibitive amount of memory. It currently works with a 100 point data set, buffered by 10 points on either end to

reduce impulse effects. Normally, the program gets the 10 buffer points from the spectrum itself, using the 10 points adjacent to the data set in use. If the data set in use is the first data set in the spectrum, Subroutine RBUFF1 creates a buffer of 10 points by applying an exponential decay to the first point in the data set, after considering the slope of the spectrum at that point. Subroutine RBUFF2 performs the same function on the trailing end of the last data set in the spectrum. It should be noted that 100 point data sets are unrealistically small for most spectroscopic applications. The size was chosen initially to minimize the computer time used in the development phase; the extension to larger blocks is straightforward.

Subroutine REUFF reads the spectrum into memory using the 120 point data sets--100 points of working data and 20 points of buffer data. To illustrate the function of the program, one data set will be tracked through its processing.

First, subroutine LSQ smoothes the data set using a nine-point quadratic least-squares fit. The fit leads to a 3×3 matrix that is solved by gaussian elimination. During the gaussian elimination, LSQ checks the matrix of coefficients calculated for the least-squares fit to ensure that the multiplier used to reduce the matrix is

less than unity. If necessary, LSQ calls subroutine INVERT. INVERT pivots the matrix to reduce error propagation by insuring that all multiplications are by factors less than one.

The next step is the actual filter application. Subroutine FILTER uses a non-recursive filter generated from a least-squares prediction for two points on either side of the n th point. The filter weights the predictions for the n th point based on the number of data points separating the prediction from the n th point. The predictions two points away are weighted by a factor of 0.1, those one point away are weighted by 0.2 and the prediction at the n th point is weighted 0.4. Figure 3 depicts the filtering scheme used for the interior points.

Next, FILTER shifts one point to the right and repeats the process for the next point, producing a "moving average." It should be noted that the end points of the data set have a different weighting scheme which is enumerated in the source code, however, points calculated with that different weighting scheme are all discarded when the buffer points are stripped from the data set.

After the filter application, subroutine WBUFF strips the 20 buffer points from the data set and sequentially writes the 100 working data points to a temporary

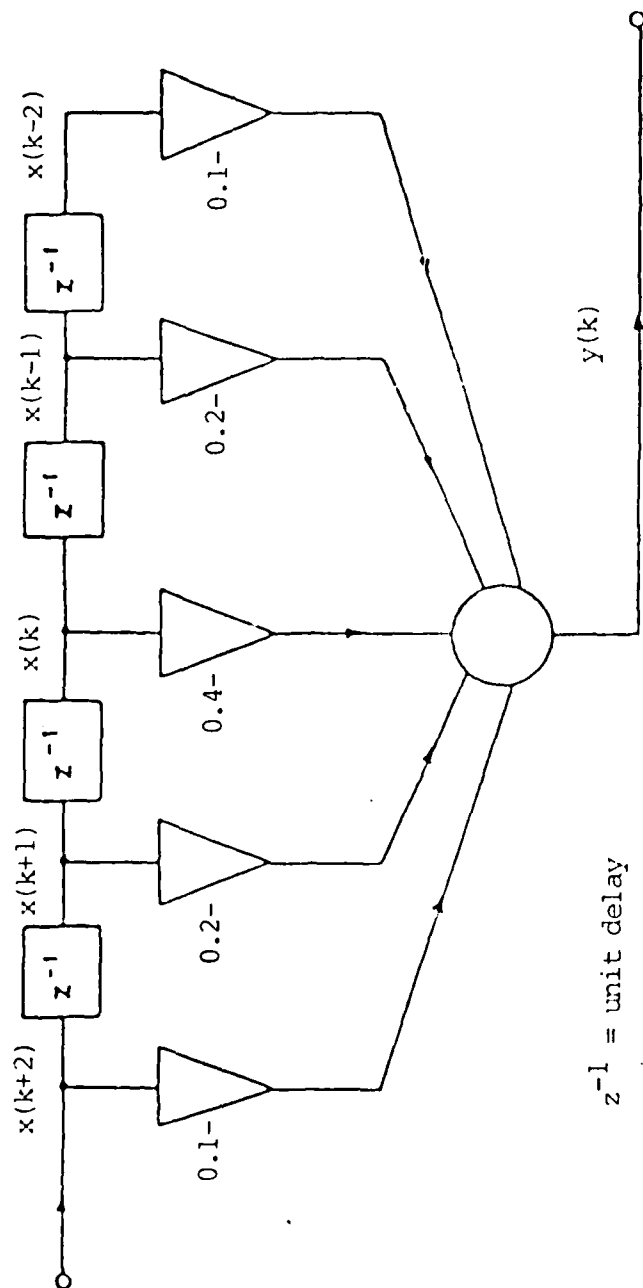


Figure 3. Diagram of the filtering scheme used by FILTER.

holding file. Once the working data set is written to its holding file, its existence as a data set is complete.

The program loops back to subroutine RBUFF to begin the process for the next data set in the spectrum. The cycle continues until there are no more 100 point data sets remaining in the spectrum.

When processing is complete for the observed spectrum, the program begins processing the calculated spectrum, repeating the entire process that was performed on the observed spectrum for the calculated spectrum.

With each spectrum in its respective holding file, subroutine MINUS reads the processed observed spectrum and the processed calculated spectrum into memory and subtracts the calculated spectrum from the observed spectrum point-by-point to get the residual error spectrum.

Finally, before the program terminates, an option to subtract an additional calculated spectrum is offered.

A cursory error trapping function is included in subroutine ERROR. If an error is detected by RBUFF while reading a spectrum file, ERROR issues a warning that the error was encountered. It should be noted that ERROR does not check the validity of the input data and the program does not terminate if an error is encountered. The sole purpose of ERROR is to caution the user that his residual spectrum is probably inaccurate. If ERROR

issues a warning, the user should check the data files for proper format. The error code issued by ERROR is machine specific and must be interpreted by the user based on the local machine installation.

CHAPTER IV

RESULTS

Testing Using Simulated Data

Since the concept of the program is new, testing presented a problem. There are no known spectra with which to compare the results to determine that a valid solution has been achieved. Consequently, a "known" spectrum was created for testing purposes.

First two individual stick spectra, called DA and DB, were created with a pseudo-random number generator. Line positions were randomly determined; then a random intensity was matched against each line position. A third spectrum, D2, was created by combining the first two. Finally, each spectrum was convolved with a Gaussian whose FWHM was seven data points to simulate the combined effects of the natural line width, Doppler broadening, pressure broadening, and the instrument function. The convolved spectra are called GA, GB and G2 respectively.

The final G2 spectrum then contained two, and only two, known components. If FILTER was applied to remove GA from G2, the resultant should have been GB. The results are illustrated in Figures 4-7. A further check was made by removing the calculated GB from the residual

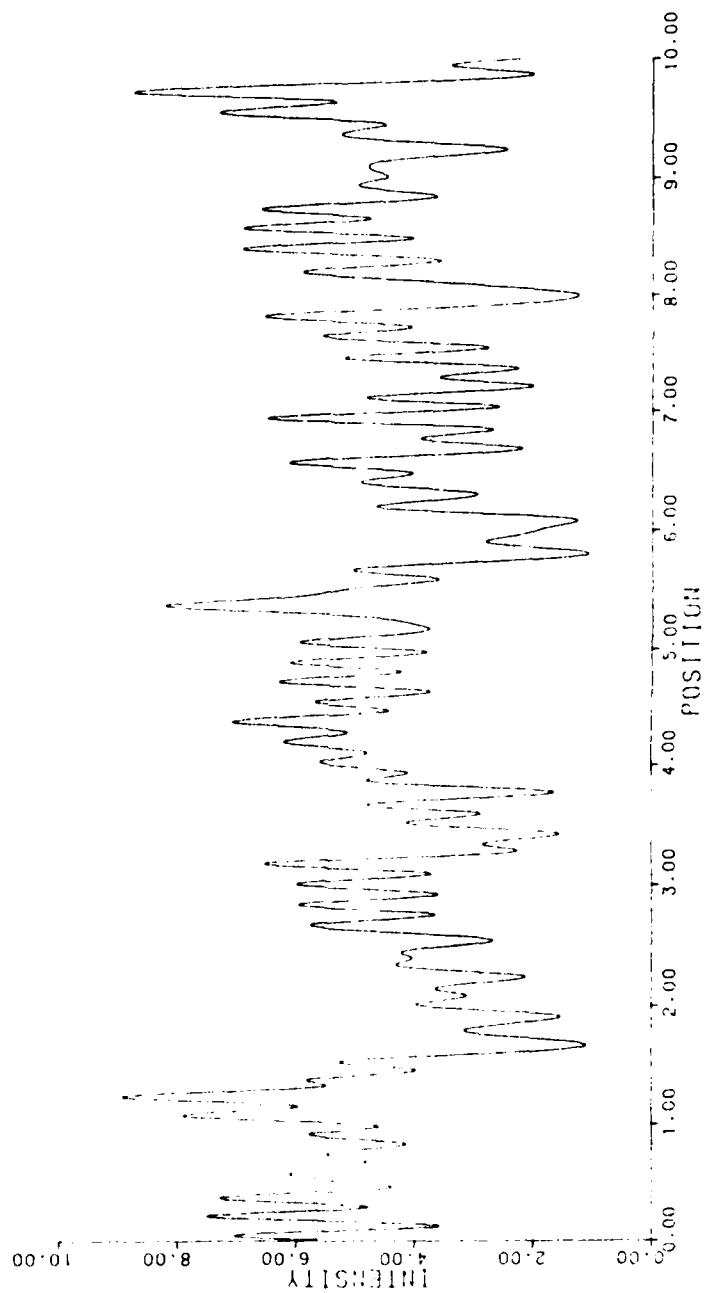


Figure 4. Plot of GA.

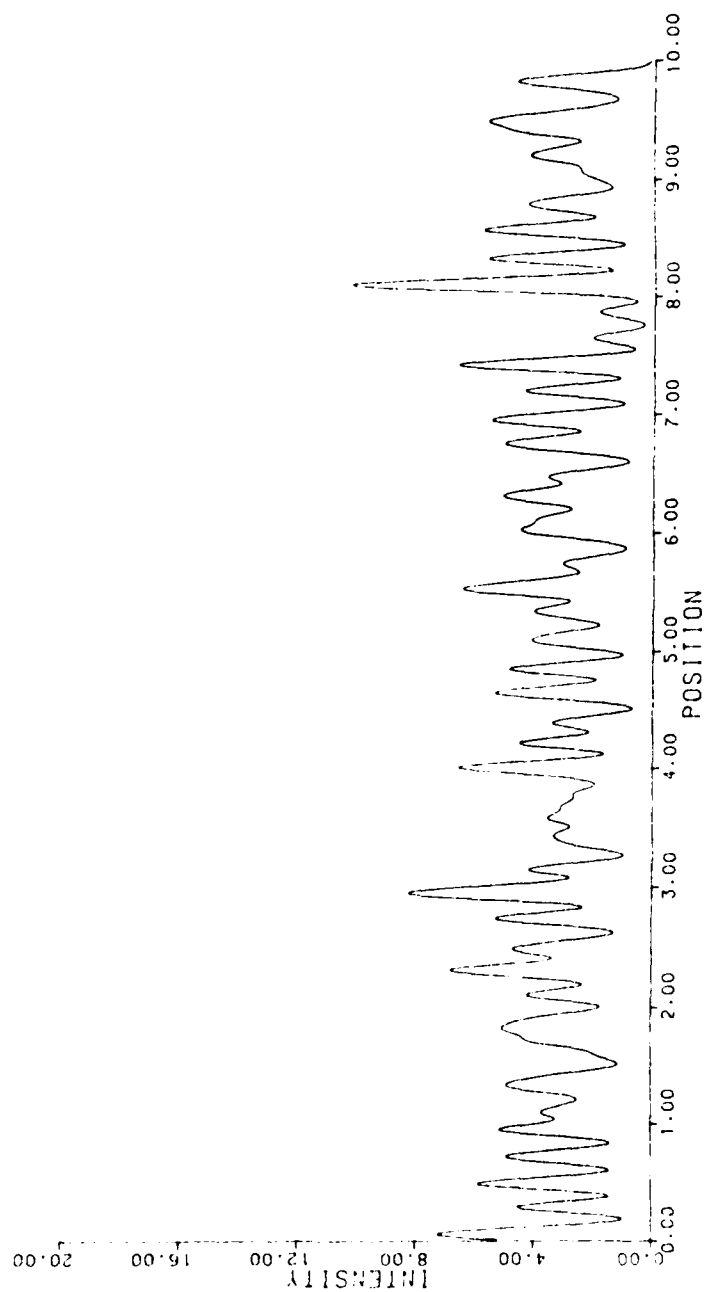


Figure 5. Plot of GB.

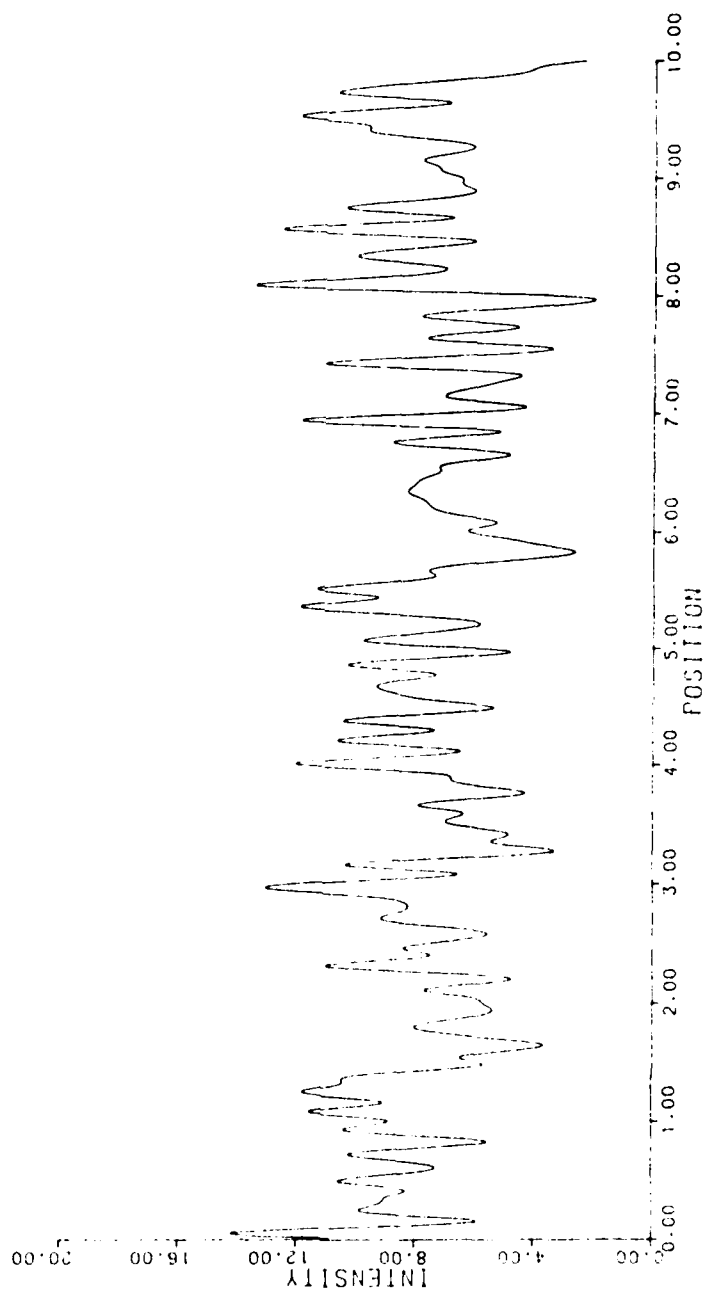


Figure 6. Plot of G2.

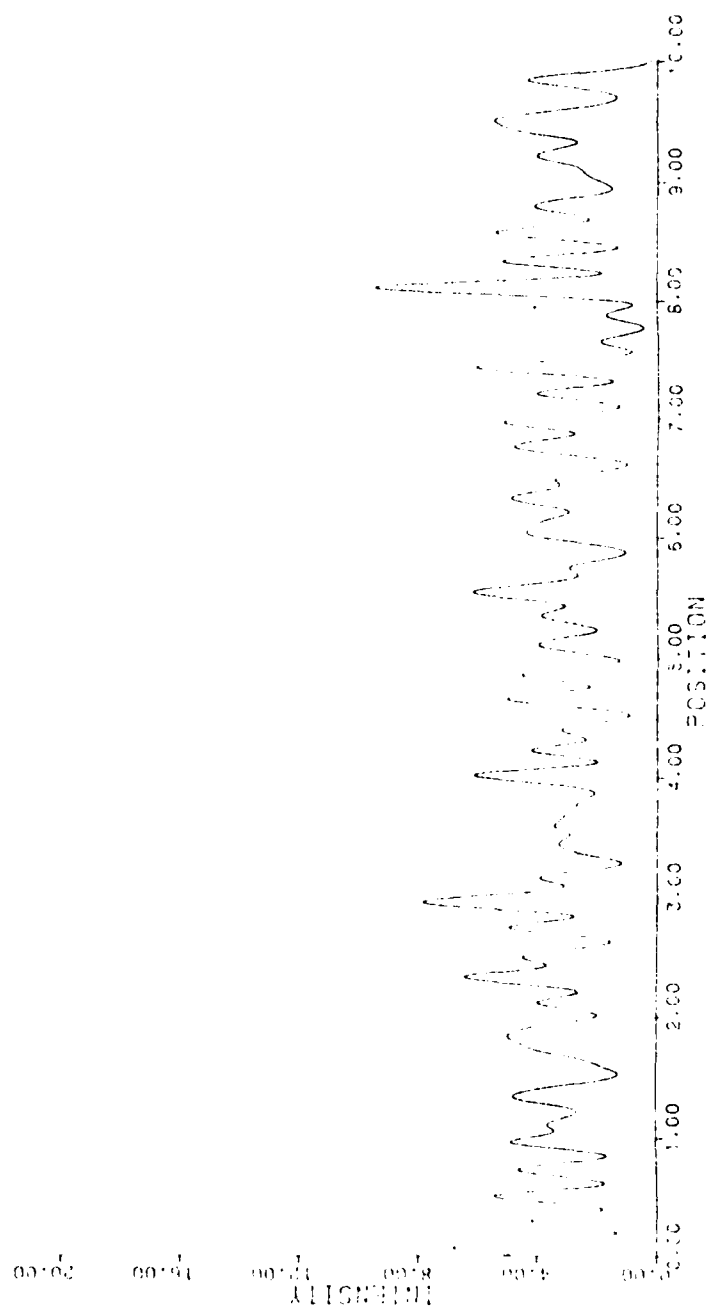


Figure 7. Plot of G2 - GA.

of $G2 - GA$ (for convenience, the act of removing one spectrum from another will be denoted by "-"). The final result was an error spectrum whose peak intensity was on the order of 1.0×10^{-6} .

To complicate the picture, a "noise" spectrum was generated, added to the stick spectrum D2 and convolved with the Gaussian. The noise spectrum was generated using a pseudo-random number generator similar to the one used to generate DA and DB. The resultant spectrum was scaled to give a signal-to-noise ratio of approximately 20:1. After removing GA from the new G2, the result was GB to within the noise. $G2 - GA$ is illustrated in Figure 8.

The final step in the testing phase was to add a single line to the D2 stick spectrum that contained the additional noise spectrum. The intensity of the line was approximately 10% of the average local intensity and approximately twice the average local noise level. This new G2 spectrum was then convolved with the Gaussian, and FILTER was used to remove GA and GB. The resultant spectrum faithfully retained the added line and removed all other lines above the noise. See Figure 9.

Actual Data Runs

After validating the basic concept, FILTER was used to remove the calculated ν_9 band of ethane from the

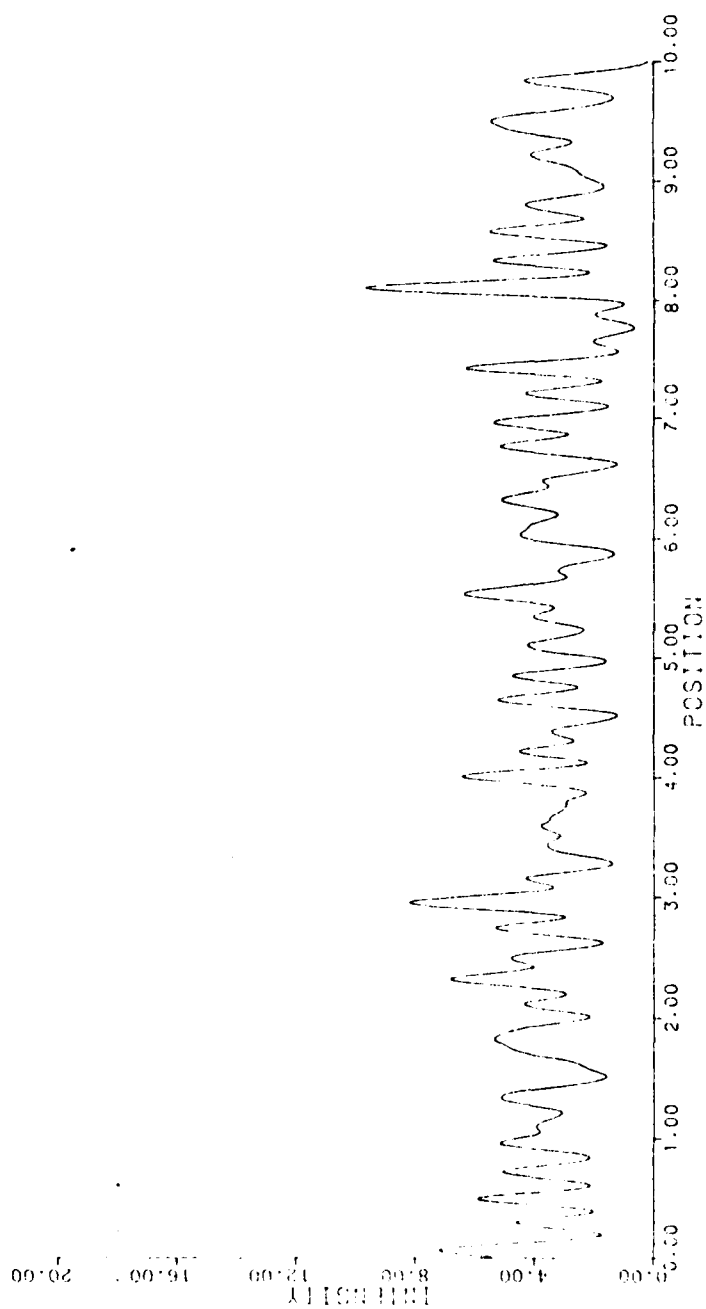


Figure 8. Plot of G2 - GA with noise included.

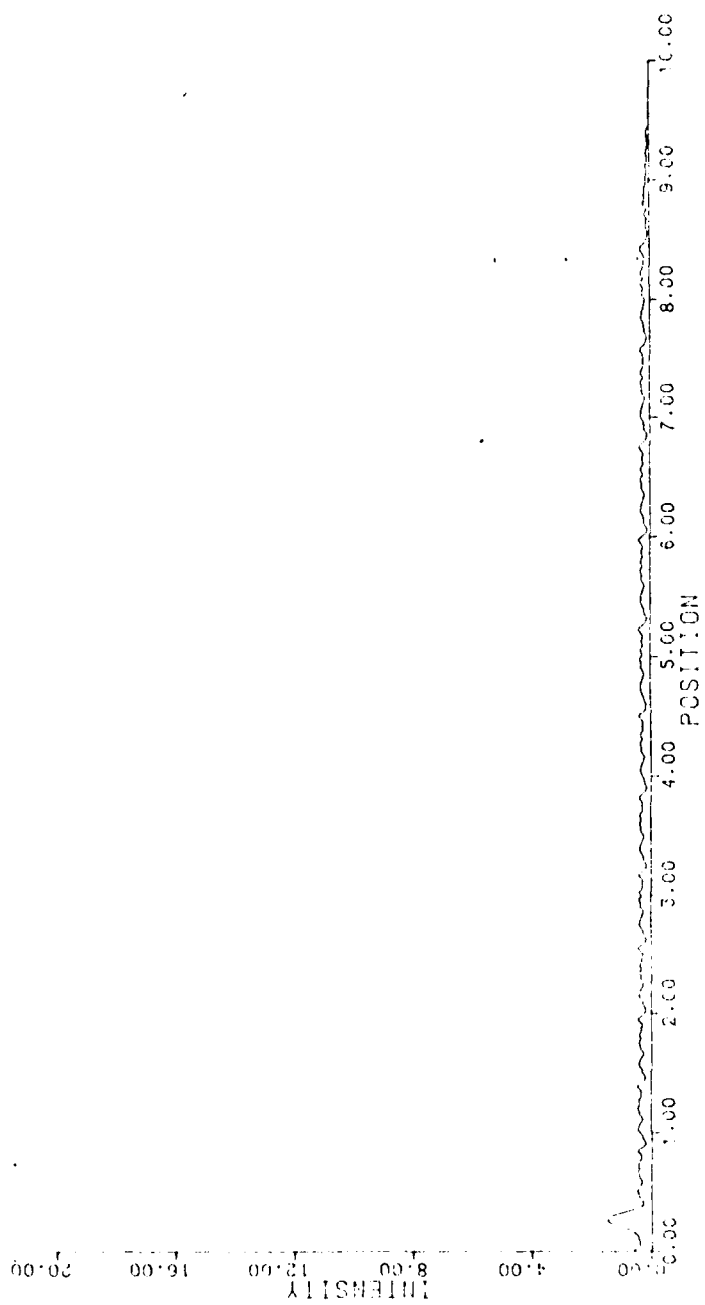


Figure 9. Plot of G2 (with test feature added) - GA - GB.

observed ethane spectrum at three different frequencies. The frequencies were chosen to represent three different levels of activity: one with low activity near 815.0 cm^{-1} , another with some activity but little expected hot-band activity near 804.0 cm^{-1} , and a final one with a great deal of cold-band activity and hot-band activity near 819.5 cm^{-1} .

The segments of the observed ethane spectrum used were recorded on the one-meter Fourier transform spectrometer (FTS) at the McMath solar telescope at Kitt Peak National Observatory (Jennings, 1984). This is similar to data taken by Daunt *et al.* (1984) except the resolution was doubled to approximately 2.5 milli-wavenumbers by modifying the FTS to double pass the interferometer. The calculated stick spectrum used is taken from data by Atakan *et al.* (1983).

In computing the theoretical spectrum, it was found that a factor of $12.1 \times 10^{-3} \text{ cm}^{-2} \text{ atm}^{-1}$ was necessary to convert the relative intensities given in the spectral catalog to absolute intensities. The doppler width was calculated to be 1.8 milli-wavenumbers and the pressure width, 0.5 milli-wavenumbers. The instrument function for the FTS was taken to be a sinc function with FWHM of 3.0 milli-wavenumbers. The observed, calculated and resultant spectra are illustrated in Figures 10-18.

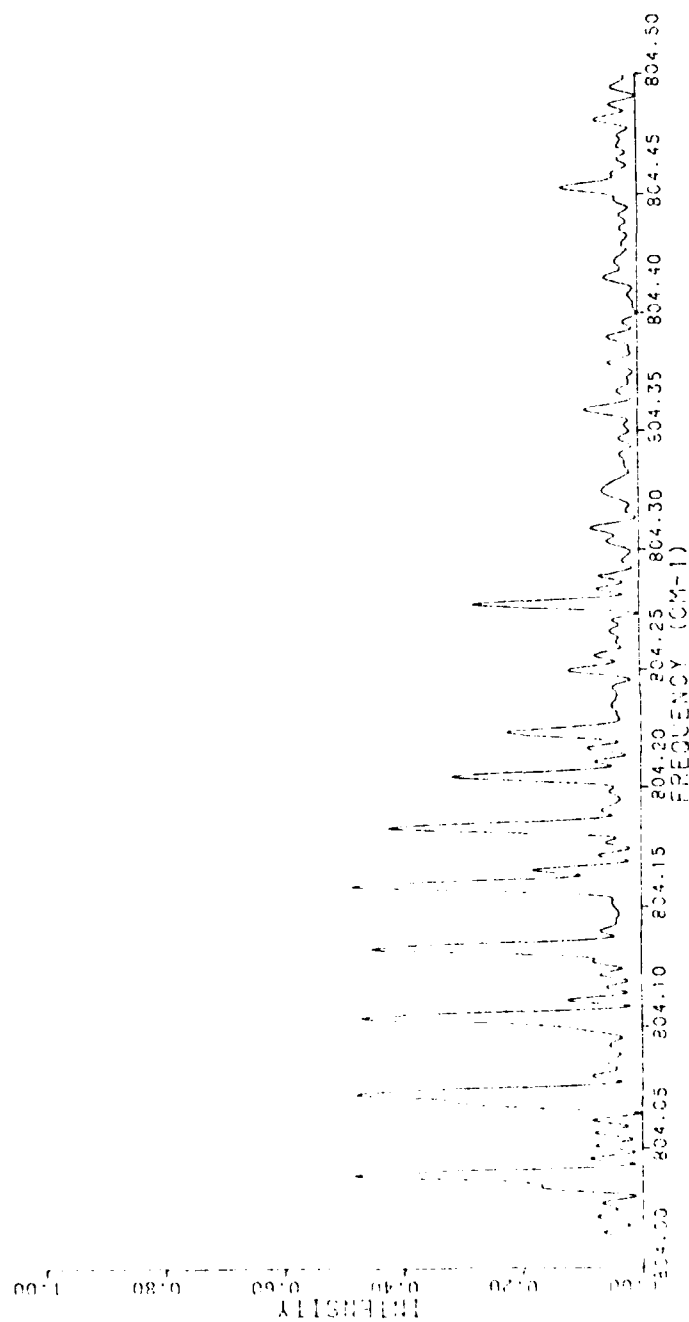


Figure 10. Portion of the observed spectrum of ethane near 804.0 cm^{-1} .

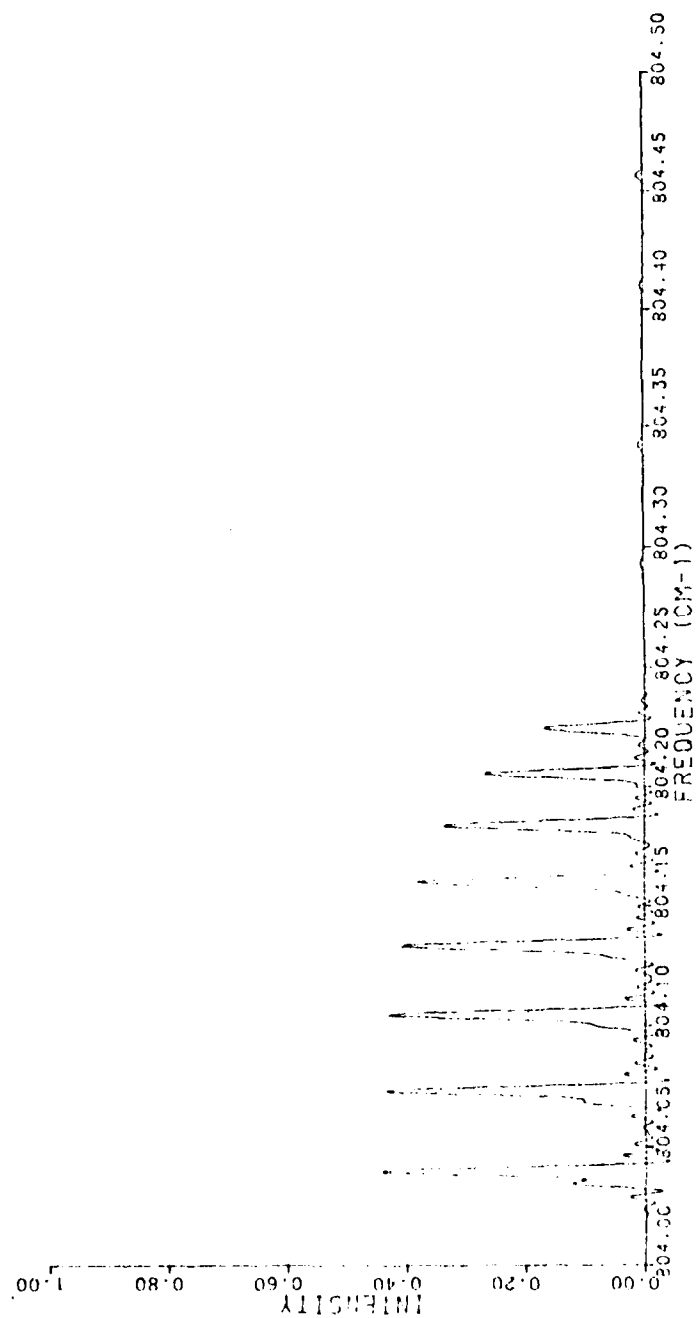


Figure 11. Calculated ν_g band of ethane near 804.0 cm^{-1} .

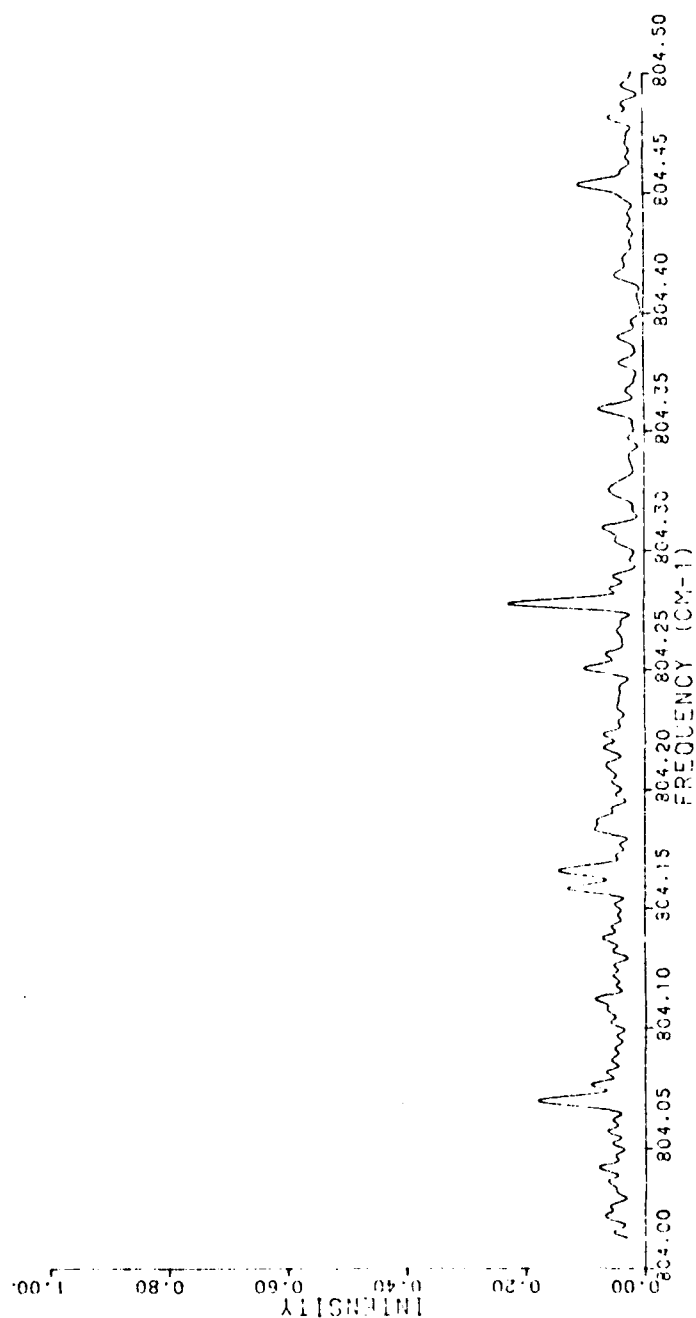


Figure 12. Residual spectrum near 804.0 cm⁻¹ generated by FILTER.

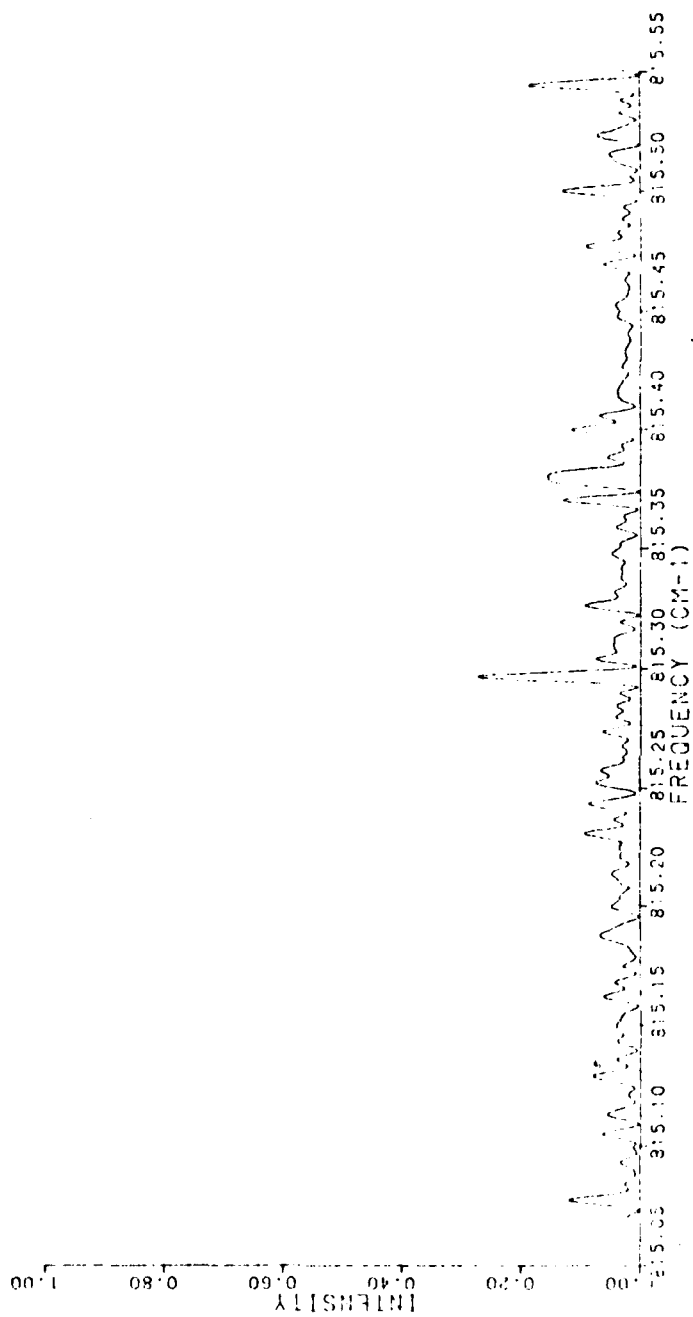


Figure 13. Portion of the observed spectrum of ethane near 815.0 cm^{-1} .

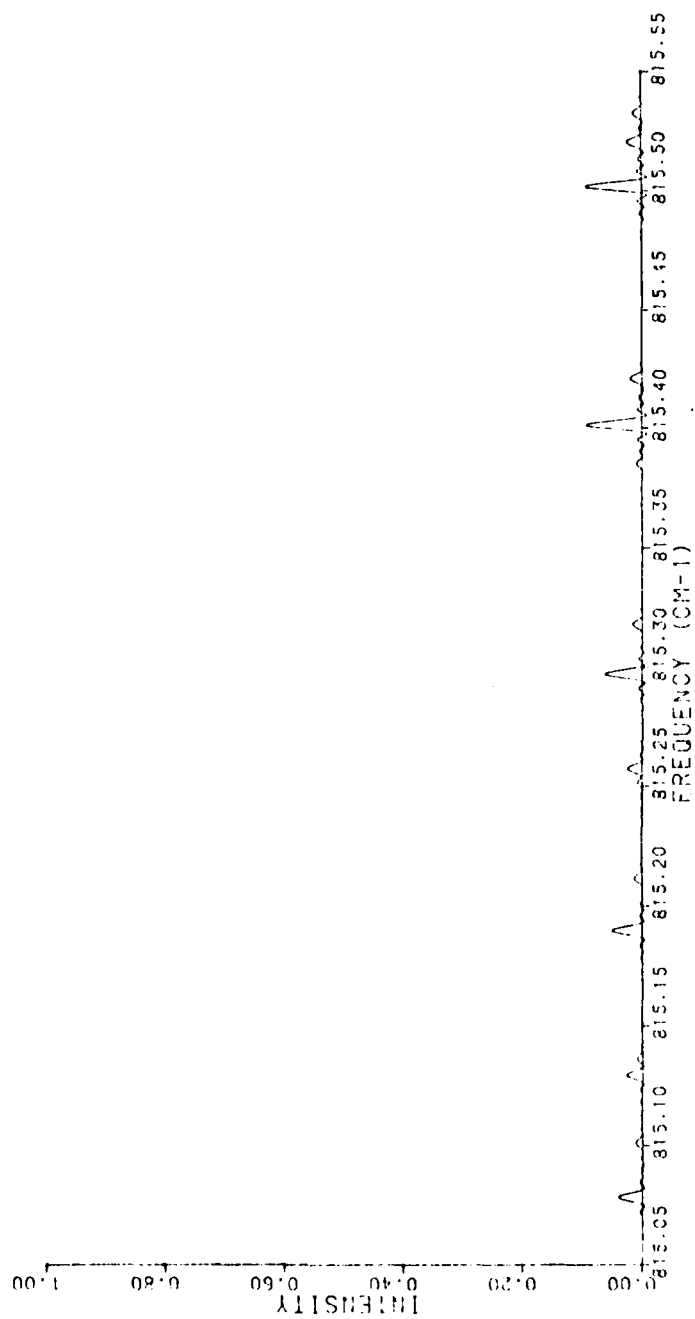


Figure 14. Calculated ν_9 band of ethane near 815.0 cm^{-1} .

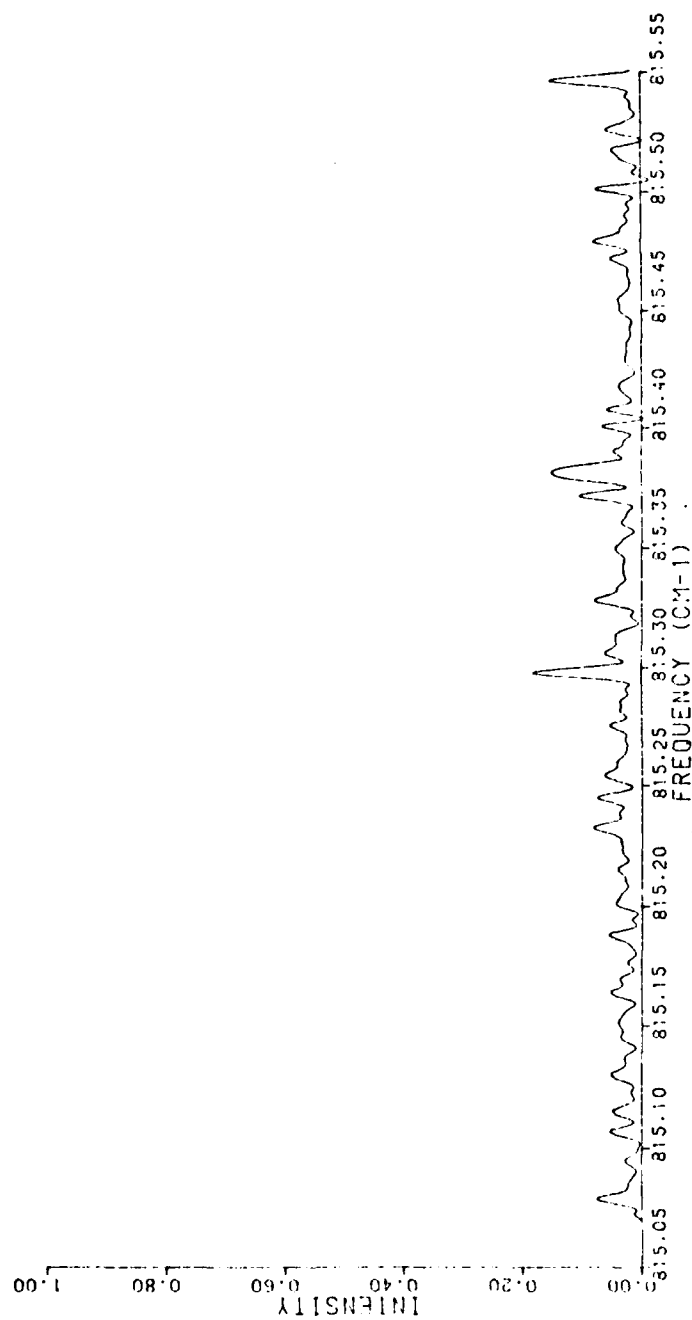


Figure 15. Residual spectrum near 815.0 cm^{-1} generated by FILTER.

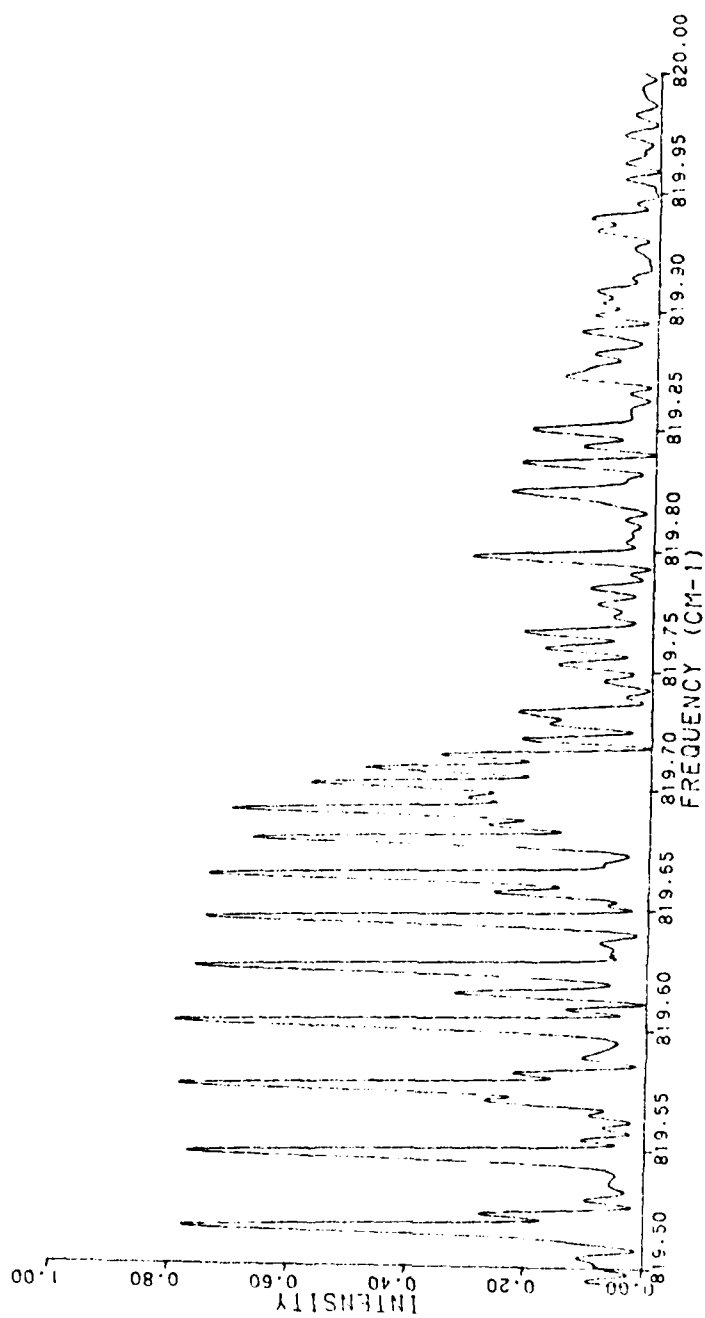


Figure 16. Portion of the observed spectrum of ethane near 819.5 cm^{-1} .

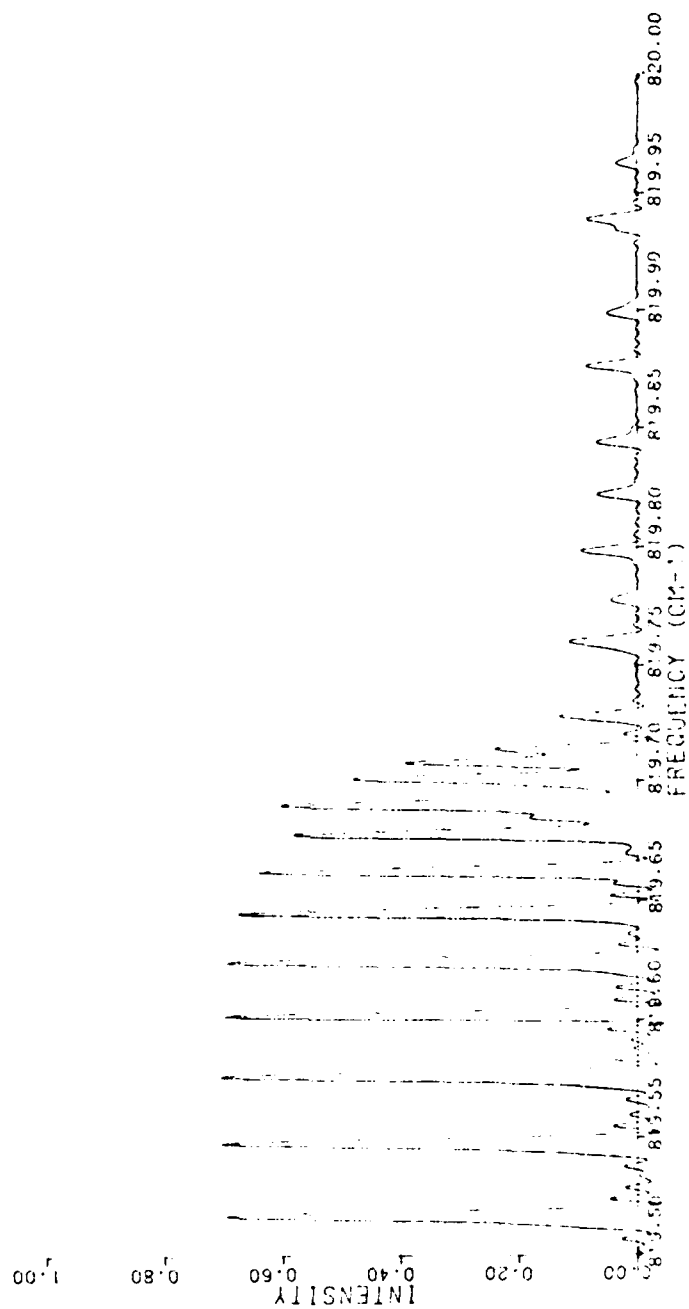


Figure 17. Calculated ν_g band of ethane near 819.5 cm^{-1} .

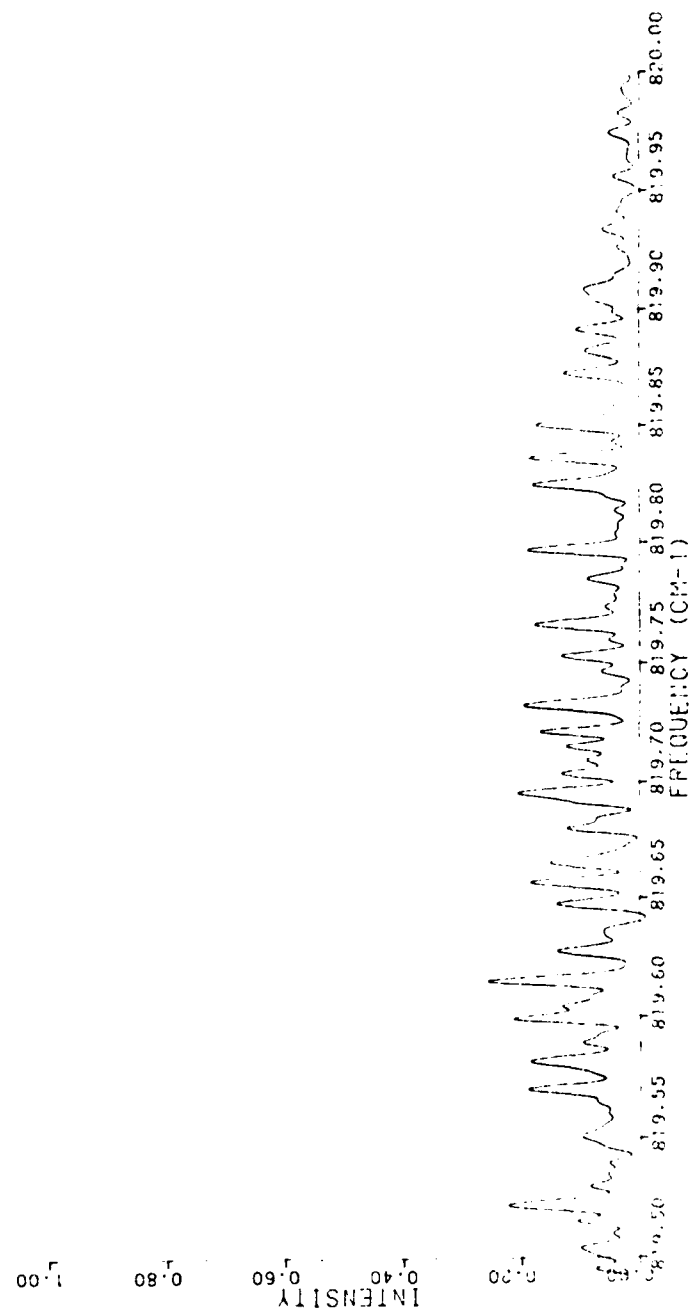


Figure 18. Residual spectrum near 819.5 cm^{-1} generated by FILTER.

As an additional cross check of the validity of the resultant data, one very small line was removed from the calculated stick spectrum at $819.66089 \text{ cm}^{-1}$. The continuous spectrum calculated from this new stick spectrum is shown in Figure 19, with the position of the removed line indicated by an asterisk (*). The error spectrum produced by using the new continuous spectrum in FILTER is identical to the error spectrum produced by using the original stick spectrum except for the reappearance of the single line. The line is identified with an asterisk (*) in Figure 20.

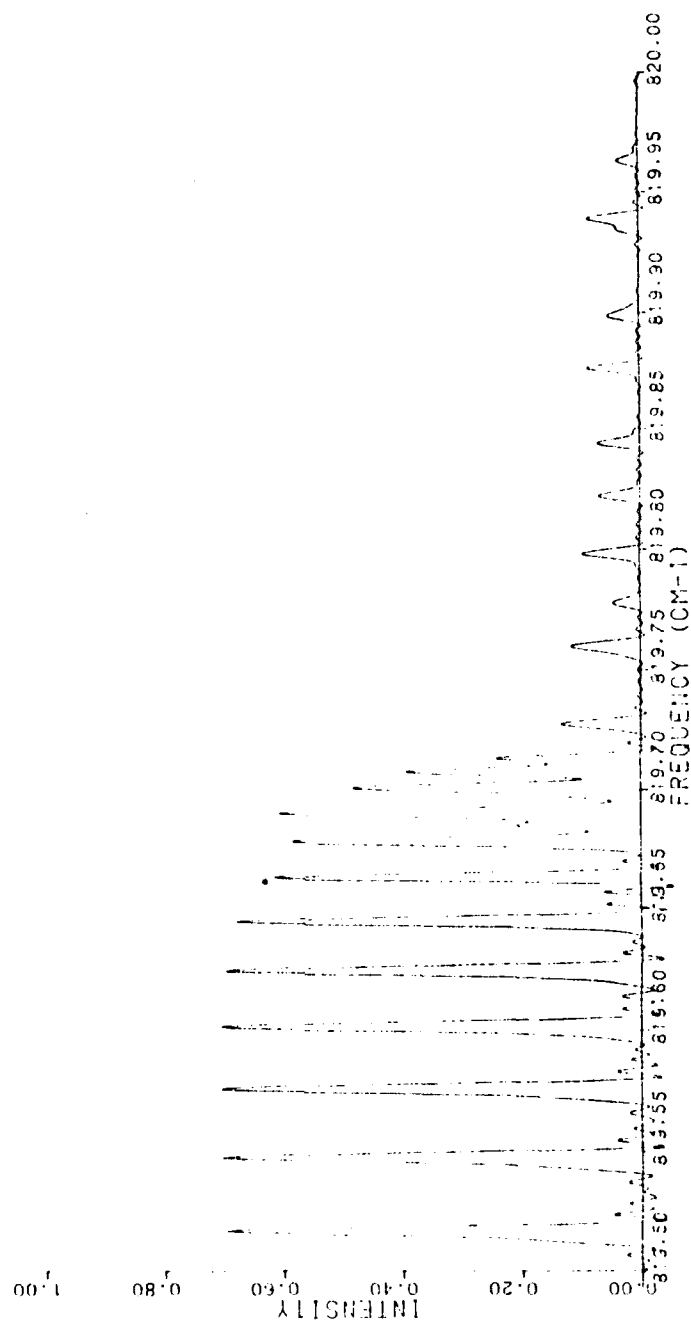


Figure 19. Calculated ν_g band of ethane near 819.5 cm^{-1} with a line removed at $819.66089 \text{ cm}^{-1}$.

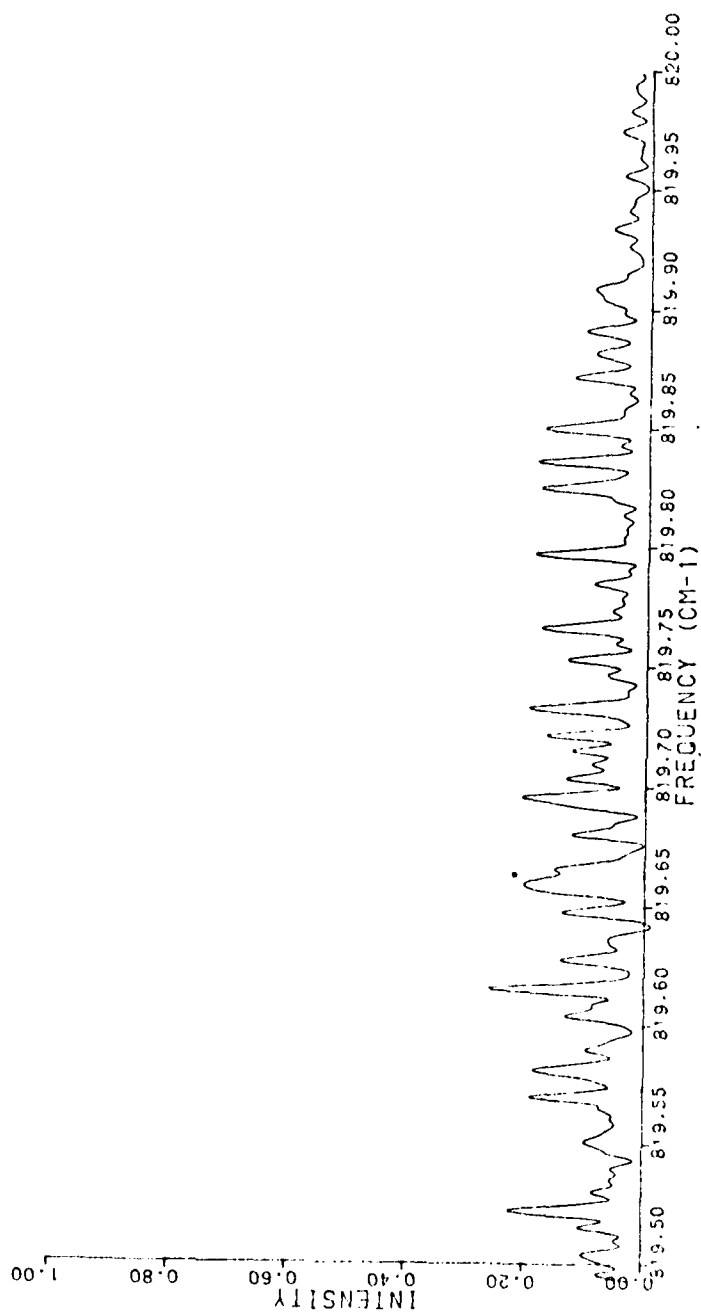


Figure 20. Residual spectrum generated by FILTER without the line at $819.66089 \text{ cm}^{-1}$.

CHAPTER V

DISCUSSION

The spectra used in the testing phase are fully known since they were created specifically for testing. Consequently, evaluation of the program function is fairly objective. G2 with GA and GB removed is effectively zero. Furthermore, when G2 contains features not in GA or GB, those extra features remain when GA and GB are removed. Hence, one can say the procedures employed by FILTER are correct for the intended purpose.

When considering real spectral data, the interpretation of the results is definitely more subjective; there is no reliable predictor of the residual spectrum.

Before evaluating the program's effectiveness with observed spectra, one must ensure that the observed spectrum and the theoretical spectrum truly represent the same data. That is, each data point in the observed spectrum must be exactly equivalent to the corresponding data point in the calculated spectrum. Failure to properly match the spectra will generate some oscillatory behavior or large negative excursions by mismatching peak positions. Neither condition is desirable and any negative absorption is clearly non-physical. To ensure that the data is in fact equivalent, the starting frequencies

must exactly coincide and the data-point density, or the step size, must also be the same.

Furthermore, when converting the calculated stick spectrum to a continuous theoretical spectrum as in Equation (12), Page 11, the line shape chosen to convolve with the stick spectrum will affect the peak intensities of the calculated spectrum. A normalized line shape preserves the total energy, but in doing so it necessarily reduces the peak intensity by spreading the energy over a wider frequency range. In the present work, the absorption coefficient was calculated

$$\alpha = (D \otimes P) S_0$$

where S_0 is the absolute line strength determined from data by Atakan et al. (1983) as

$$S_0 = 7.1 \times 10^{-3} S_R$$

where S_R is the published relative line strength.

Using data supplied by Jennings (1984) of 1.5 torr pressure, 296°K temperature, and 150 cm path length, it was found that the intensities of the calculated spectrum were too low by a factor of 1/3 to effectively remove their contribution from the observed spectrum. In order to bias the intensities of the calculated spectrum to match those of the observed spectrum, a factor of 12.1 x

$10^{-3} \text{ cm}^{-2} \text{ atm}^{-1}$ was used in converting the calculated relative intensities to absolute intensities.

The discrepancy between the expected and actual conversion factor can be ascribed to inaccuracy in the measurement of the pressure of the sample (Jennings, 1984). If one assumes the given value of 7.1×10^{-3} is correct, the discrepancy corresponds to an actual pressure of 2.6 torr. Additionally, the discrepancy may be a result of inaccuracies in establishing the base line (Blass, 1985). Obviously, any combination of the two errors could account for the discrepancy.

The natural question arising is "How does one decide that the calculated spectrum is a good predictor of the known part of the observed spectrum?"

By looking at a section of the spectrum with relatively little activity, one may make an educated guess at the reliability of the residual spectrum. Presumably, most of the lines will be completely eliminated by the filter, leaving noise. The spectrum near 815.0 cm^{-1} demonstrates that FILTER will remove those components when there is not much underlying activity.

For the more active sections of the spectrum, a comparison of the calculated spectrum with the observed spectrum can be used to determine that a given line has been completely removed from the residual spectrum. In such a case, care must be exercised not to confuse an

underlying element of the observed spectrum that should properly exist in the residual spectrum with a portion of the calculated spectrum that was not completely removed by FILTER. The spectrum near 804.0 cm^{-1} includes a segment of fairly high spectral activity followed by a segment of relatively little activity showing that FILTER will remove the known components in a region of high spectral activity without altering the underlying data. The spectrum near 819.5 cm^{-1} is an extremely busy portion of the ethane spectrum, complete with hot-band activity underlying the ground-state transitions, yet FILTER effectively removed the ground-state transitions, leaving what is presumed to be hot-band transitions. Analysis of the residual spectrum is left for further study.

Whether to deconvolve the data before applying this program is a question to be answered before the data is taken. Expected resolution of the experimental data or an unreasonably long observation are factors to consider, but the use of FILTER is not dependent on the existence of deconvolved data. However, the effect that FILTER may have on the deconvolution process has not yet been investigated, and the very strong sensitivity of the deconvolution process to the signal-to-noise ratio of the data suggests that deconvolution should be performed before the algorithm in FILTER is applied.

APPENDIX

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PROGRAM LISTING

```

C*****
C*                                PROGRAM FILTER                                *
C*****
C
C THIS PROGRAM ACTS AS A FILTER TO REMOVE KNOWN COMPONENTS FROM A
C DIGITAL SPECTRUM. IT SMOOTHS THE SPECTRA USING A QUADRATIC
C LEAST SQUARES FIT WHERE NFIT*2+1 IS THE NUMBER OF POINTS IN THE LEAST
C SQUARES FIT, THEN IT USES THE TWO POINTS ON EITHER SIDE OF A POINT AND
C THE SAME POINTS IN THE CALCULATED SPECTRUM TO MAKE A PREDICTION FOR EACH
C POINT IN THE SPECTRUM. TO ACCOMMODATE LARGE SPECTRA, A BUFFERING ROUTINE
C IS USED TO WORK WITH SECTIONS OF THE SPECTRA INDIVIDUALLY. IT CURRENTLY
C USES 100 DATA POINTS BUFFERED BY 10 DATA POINTS ON EITHER END.
C
      DIMENSION XINT1(120),XINT2(120),A1(120),A2(120)
      DIMENSION B1(120),B2(120),C1(120),C2(120),FILE1(6),FILE2(6)
      DOUBLE PRECISION XINT1, XINT2, A1, A2,B1,B2,C1,C2
      COMMON NDATA,NFIT,NBUFF,NFLAG
C
C NDATA IS THE DATA SET SIZE PLUS THE TOTAL NUMBER OF BUFFER POINTS
C
      NDATA=120
C
C NBUFF AND NFLAG ARE FLAGS USED BY SUBROUTINES
C
      NBUFF=0
      NFLAG=0
C
C ISIZE IS THE ESTIMATED SIZE OF THE SPECTRA/10 + 1. IT IS USED
C AS A LIMIT TO PREVENT AN INFINITE LOOP
C
      ISIZE=11
C
C NFIT*2+1 = THE NUMBER OF POINTS USED IN THE SMOOTHING
C
      NFIT=4
      WRITE (5,100)
100  FORMAT(' INPUT FILESPEC FOR THE MAIN SPECTRUM')
      READ (5,200) FILE1
200  FORMAT (6A5)
      DO 20 I=1,ISIZE
          CALL RBUFF(XINT1,FILE1,INT)
          IF (INT+10.LT.NDATA) NDATA=INT+10
          CALL LSQ(XINT1,A1,B1,C1)
          CALL FILTER(XINT1,A1,B1,C1)
          CALL WBUFF(XINT1,FILE1,INT)
          IF (NFLAG.EQ.1) GO TO 30
20    CONTINUE
30    WRITE (5,400)
400  FORMAT (' INPUT FILESPEC OF THE SPECTRUM TO BE SUBTRACTED')
      READ (5,200) FILE2
C
C REINITIALIZE THE FLAGS
C
      NBUFF=0
      NFLAG=0
      DO 40 I=1,ISIZE
          CALL RBUFF(XINT2,FILE2,INT)
          IF (INT+10.LT.NDATA) NDATA=INT+10
          CALL LSQ(XINT2,A1,B1,C1)
          CALL FILTER(XINT2,A1,B1,C1)
          CALL WBUFF(XINT2,FILE2,INT)
          IF (NFLAG.EQ.1) GO TO 50
40    CONTINUE
50    CALL MINUS(FILE1,FILE2,INT)

```

```

C
C OFFER OPTION TO REMOVE MORE FROM THE SPECTRUM
C
      WRITE (5,500)
500   FORMAT (' IS THERE ANOTHER SPECTRUM TO BE SUBTRACTED? 1=YES')
      READ (5,600) LOOP
600   FORMAT (I1)
      IF (LOOP.EQ.1) GO TO 30
      WRITE (20,300) XINT1
300   FORMAT (D20.12)
      END
C*****
      SUBROUTINE LSQ(Y,A,B,C)
C*****
C
C THIS SUBROUTINE MAKES A QUADRATIC LEAST SQUARES FIT TO
C A DIGITAL SPECTRUM. NDATA IS THE NUMBER OF DATA POINTS.
C NFIT*2+1 IS THE NUMBER OF POINTS IN THE LEAST SQUARES FIT
C
      COMMON NDATA,NFIT
      DIMENSION MATRIX(3,4), Y(NDATA), A(NDATA), B(NDATA), C(NDATA)
      DOUBLE PRECISION MATRIX, Y, A, B, C, MULT
      DO 10 N=1,NDATA

C
C INITIALIZE THE MATRIX ELEMENTS
C
      SX1=0.
      SY1=0.
      SX2=0.
      SX3=0.
      SX4=0.
      SX1Y1=0.
      SX2Y1=0.
      XN=2*NFIT+1

C
C COMPUTE THE MATRIX ELEMENTS
C
      DO 20 M=-NFIT,NFIT
          IF (N+M-1.LT.1) GO TO 25
          IF (N+M-1.GT.NDATA) GO TO 25
          Y1=Y(N+M-1)
25         X1=FLOAT(M)
          X2=X1*X1
          X3=X2*X1
          X4=X3*X1
          X1Y1=X1*Y1
          X2Y1=X2*Y1
          SY1=SY1+Y1
          SX1=SX1+X1
          SX2=SX2+X2
          SX3=SX3+X3
          SX4=SX4+X4
          SX1Y1=SX1Y1+X1Y1
          SX2Y1=SX2Y1+X2Y1
20        CONTINUE
          MATRIX(1,1)=XN
          MATRIX(2,1)=SX1
          MATRIX(3,1)=SX2
          MATRIX(1,2)=SX1
          MATRIX(2,2)=SX2
          MATRIX(3,2)=SX3
          MATRIX(1,3)=SX2
          MATRIX(2,3)=SX3
          MATRIX(3,3)=SX4
          MATRIX(1,4)=SY1
          MATRIX(2,4)=SX1Y1
          MATRIX(3,4)=SX2Y1

```

```

C
C CHECK THE SIZE OF THE MATRIX ELEMENTS
C
      DO 30 I=1,2
        DO 40 J=1,3
          I1=I
          J1=J
        C
        C IF THE MULTIPLIER WOULD BE > 1, PIVOT THE MATRIX
        C
          IF (ABS(MATRIX (I,I)).LT.ABS(MATRIX(J,I)
            ))CALL INVERT(I1,J1,MATRIX)
          1
          CONTINUE
        C
        C COMPUTE THE REDUCED MATRIX
        C
          DO 50 J=I+1,3
            MULT=-MATRIX(J,I)/MATRIX(I,I)
            DO 60 K=1,4
              MATRIX(J,K)=MATRIX(J,K)+
                MULT*MATRIX(I,K)
            1
            CONTINUE
          60
          50
          30
          CONTINUE
        C
        C CALCULATE THE VALUES OF THE COEFFICIENTS
        C
          C(N)=MATRIX(3,4)/MATRIX(3,3)
          B(N)=(MATRIX(2,4)-C(N)*MATRIX(2,3))/MATRIX(2,2)
          A(N)=(MATRIX(1,4)-B(N)*MATRIX(1,2)-C(N)*MATRIX(1,3))
            /MATRIX(1,1)
          1
          CONTINUE
        10
        RETURN
        END
      C
      C*****
      SUBROUTINE INVERT(I,J,MATRIX)
      C*****
      C
      C THIS SUBROUTINE PIVOTS THE MATRIX TO REDUCE ERROR PROPAGATION.
      C
        DIMENSION MATRIX(3,4)
        DOUBLE PRECISION MATRIX, SMALL
        DO 10 K=1,4
          SMALL = MATRIX(I,K)
          MATRIX(I,K) = MATRIX(J,K)
          MATRIX(J,K) = SMALL
        10
        RETURN
        END
      C
      C*****
      SUBROUTINE FILTER(Y,A,B,C)
      C*****
      C
      C THIS SUBROUTINE MAKES A PREDICTION FOR THE NEXT POINT BASED ON THE
      C COEFFICIENTS CALCULATED FOR THE FOUR POINTS AROUND IT.
      C
        DIMENSION Y(NDATA),A(NDATA),B(NDATA),C(NDATA)
        COMMON NDATA, NFIT
        DOUBLE PRECISION Y,A,B,C
        IEND=NDATA-2
      C
      C THE END POINTS HAVE A DIFFERENT WEIGHTING
      C
        Y(1)=.6*A(1)+.3*(A(2)+B(2)+C(2))+.1*(A(3)+2*B(3)+4*C(3))
        Y(2)=.2*(A(1)-B(1)+C(1))+.5*A(2)+.2*(A(3)+B(3)+C(3))+.1*(A(4)+2*
          1      B(4)+4*C(4))

```

```

        WRITE (21,100) Y(I)
10      CONTINUE
        CLOSE (21)
        NBUFF=NBUFF+1
        RETURN
100     FORMAT (D20.12)
        END
C*****
      SUBROUTINE RBUFF1(Y)
C*****
C
C THIS SUBROUTINE ADDS AN EXPONENTIAL DECAY TO THE BEGINNING OF THE SPECTRA
C SO THAT THE FILTERED SPECTRA DO NOT GET A BIG IMPULSE AFFECT ON THE ENDS
C
      DIMENSION Y(120)
      COMMON NDATA,NFIT,NBUFF
      DOUBLE PRECISION Y
      DO 10 I=110,1,-1
        Y(I+10)=Y(I)
10      CONTINUE
C
C COMPUTE THE FIRST POINT BASED ON THE SLOPE AND END POINT IN THE SPECTRUM
C
      FIRST=2.*Y(11)-Y(12)
      DO 20 I=10,1,-1
        XPOW=(-(10.-I)*(10.-I)/50.)
        Y(I)=FIRST*EXP(XPOW)
20      CONTINUE
      RETURN
      END
C*****
      SUBROUTINE RBUFF2 (Y,INT)
C*****
C
C THIS SUBROUTINE BUFFERS THE LAST DATA SET
C
      DIMENSION Y(120)
      COMMON NDATA,NFIT,NBUFF,NFLAG
      DOUBLEPRECISION Y
      NFLAG=1
C
C THE LAST POINT IS BASED ON THE SLOPE AND END POINT OF THE DATA SET
C
      YLAST=2*Y(110)-Y(109)
      DO 10 I=1,10
        XPOW=-I*I/50.
        Y(110+I)=YLAST*EXP(XPOW)
10      CONTINUE
      RETURN
      END
C*****
      SUBROUTINE ERROR( IOS)
C*****
C
C THIS SUBROUTINE IS PURELY PRECAUTIONARY, IT WARNS IF AN I/O ERROR IS
C ENCOUNTERED.
C
      WRITE (5,100) IOS
100     FORMAT(' I/O ERROR ENCOUNTERED. I/O ERROR IS ',I3)
      RETURN
      END
C*****
      SUBROUTINE MINUS(FILE1,FILE2,INT)
C*****
C
C THIS SUBROUTINE WILL READ THE TEMPORARY FILES AND THEN SUBTRACT THEM
C POINT-BY-POINT
C
      DIMENSION Y1(1000),Y2(1000),FILE1(6),FILE2(6),STOR1(2),STOR2(2)

```



```

Y(IEND+1)=.1*(A(IEND-1)-2*B(IEND-1)+4*C(IEND-1)) + .2*(A(IEND)-
1 B(IEND)+C(IEND))+.5*A(IEND+1)+.2*(A(IEND+2)+B(IEND+2)+C(IEND+2))
Y(IEND+2)=.6*A(IEND+2) + .3*(A(IEND+1)-B(IEND+1)+C(IEND+1)) +
1 .1*(A(IEND)-2*B(IEND)+4*C(IEND))
C
C MOST POINTS ARE WEIGHTED HERE 1,2,4,2,1
C
DO 10 I=3,IEND
Y1=.1*(A(I-2)-2.*B(I-2)+4.*C(I-2))
Y2=.2*(A(I-1)-B(I-1)+C(I-1))
Y3=.4*(A(I))
Y4=.2*(A(I+1)+B(I+1)+C(I+1))
Y5=.1*(A(I+2)+2.*B(I+2)+4.*C(I+2))
Y(I)=Y1+Y2+Y3+Y4+Y5
10 CONTINUE
20 FORMAT (D20.12)
RETURN
END
C*****
SUBROUTINE RBUFF(Y,FILENA,INT)
C*****
C
C THIS SUBROUTINE READS A 100 POINT PORTION OF THE SPECTRUM AND BUFFERS
C IT BY 10 POINTS ON EITHER SIDE.
C
DIMENSION Y(120),FILENA(6)
COMMON NDATA,NFIT,NBUFF,NFLAG
DOUBLE PRECISION Y
INT=0
OPEN (20,NAME=FILENA,ACCESS='DIRECT',RECL=22)
11=NBUFF*100-9
IEND=11+119
DO 10 I=11,IEND
IF (I.LE.0) GO TO 10
READ (20,100,REC=I,ERR=20,IOSTAT=IOS) Y(INT+1)
INT=INT+1
10 CONTINUE
C
C CREATE A LEADING BUFFER IF THIS IS THE FIRST DATA SET IN THE SPECTRUM
C
IF (NBUFF.EQ.0) CALL RBUFF1(Y)
CLOSE (20)
RETURN
20 IF (IOS.NE.510) CALL ERROR(IOS)
C
C CREATE A TRAILING BUFFER IF THIS IS THE LAST DATA SET IN THE SPECTRUM
C
CALL RBUFF2(Y,INT)
CLOSE (20)
100 FORMAT (D20.12)
RETURN
END
C*****
SUBROUTINE WBUFF (Y,FILENA,INT)
C*****
C
C THIS SUBROUTINE TRUNCATES THE OUTER 10 POINTS ON EACH SIDE AND WRITES
C THE REMAINDER TO DISK IN SEQUENTIAL ORDER.
C
DIMENSION Y(120),STORE(2),FILENA(6)
COMMON NDATA,NFIT,NBUFF,NFLAG
DOUBLE PRECISION Y
STORE(1)=FILENA(2)
STORE(2)='.TMP'
11=NBUFF*100+11
IEND=11+99
J=11
OPEN (21,NAME=STORE,ACCESS='APPEND')
DO 10 I=11,110

```

LIST OF REFERENCES

```

      DOUBLE PRECISION Y1,Y2
      COMMON NDATA,NFIT,NBUFF,NFLAG
      STOR1(1)=FILE1(2)
      STOR1(2)='.TMP'
      STOR2(1)=FILE2(2)
      STOR2(2)='.TMP'
      OPEN (20,NAME=STOR1,ACCESS='SEQUENTIAL')
      OPEN (21,NAME=STOR2,ACCESS='SEQUENTIAL')
      READ (20,100,END=20) Y1
20    READ (21,100,END=30) Y2
30    IEND=NBUFF*100
      REWIND (20)
      DO 10 I=1,IEND
          Y1(I)=Y1(I)-Y2(I)
10    CONTINUE
      WRITE (20,100) Y1
      CLOSE (20)
      CLOSE (21)
      RETURN
100  FORMAT (D20.12)
      END

```

VITA

Carey G. Mumford, III was born in Chattanooga, Tennessee on July 18, 1953. He attended elementary school in Knoxville and Atlanta. He graduated with high honors from Woodward Academy in College Park, Georgia on May 29, 1971. He entered the University of Tennessee in the fall of that year, graduated with honors on June 10, 1975 and was commissioned a Second Lieutenant in the United States Air Force the same day. He remained at the University of Tennessee for one year of post-graduate study.

After seven years of active service with the Air Force, Captain Mumford returned to the University of Tennessee under the sponsorship of the Air Force Institute of Technology to continue his studies. He graduated with a Master of Science in Physics in August, 1985.

Following graduation, Captain Mumford was assigned to the Air Force Weapons Lab at Kirtland Air Force Base, New Mexico where he served as Chief of Test Operations in the Aircraft and Missiles Branch of the Nuclear Technology Division.

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To the Graduate Council:

I am submitting herewith a thesis written by Carey G. Mumford III entitled "A Digital Filter for Removing Known Components from Spectroscopic Data." I have examined the final copy of this thesis for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Master of Science, with a major in Physics.

William E. Blass, Major Professor

We have read this thesis
and recommend its acceptance:

Accepted for the Council:

Vice Provost
and Dean of The Graduate School

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